



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:06 PM UTC

PDB ID : 8R4J / pdb_00008r4j
Title : Plastidial phosphorylase Pho1 from Solanum tuberosum in complex with caffeine
Authors : Koulas, S.M.; Leonidas, D.D.
Deposited on : 2023-11-13
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

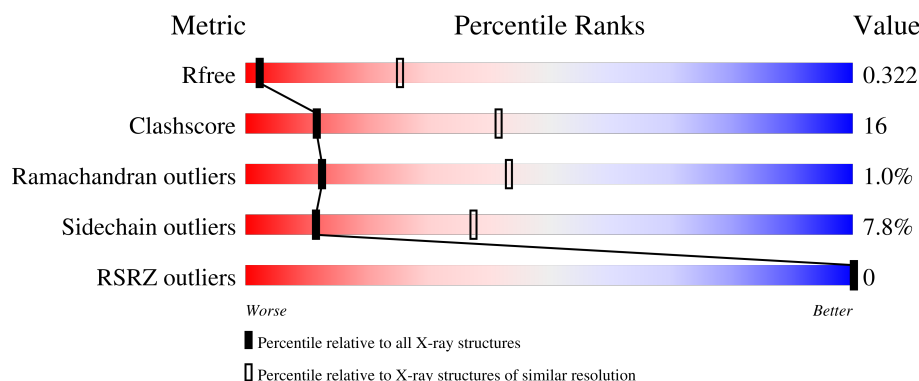
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	916	 63% 25% • 9%
1	B	916	 63% 25% • 9%
1	C	916	 59% 27% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	LLP	A	762	-	-	X	-

2 Entry composition [i](#)

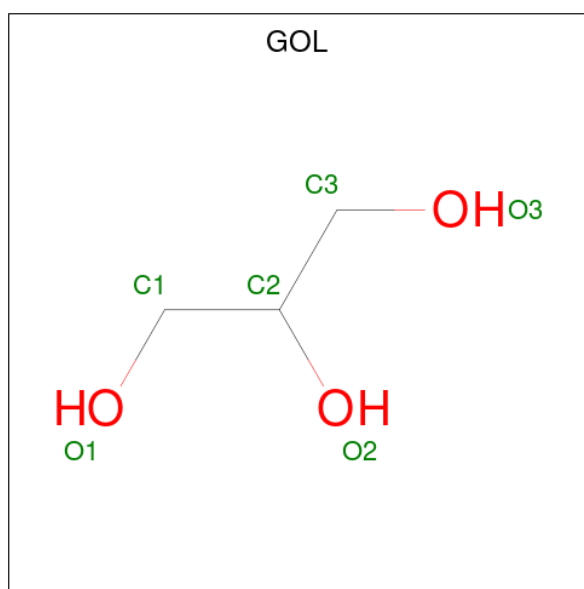
There are 4 unique types of molecules in this entry. The entry contains 20042 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/a myloplastic.

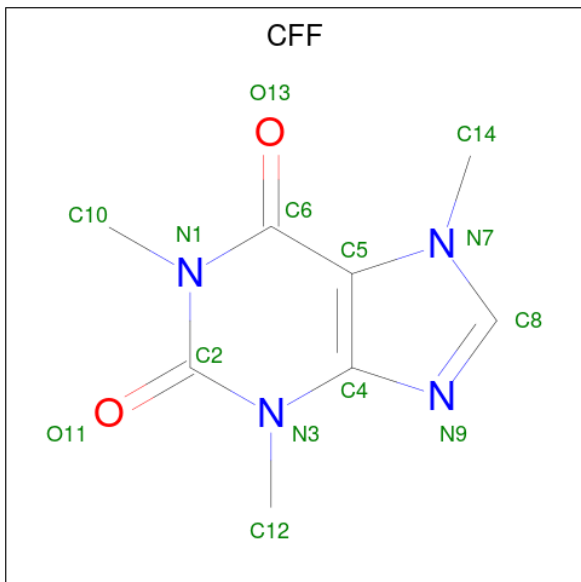
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			
1	B	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			
1	C	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	4	2		

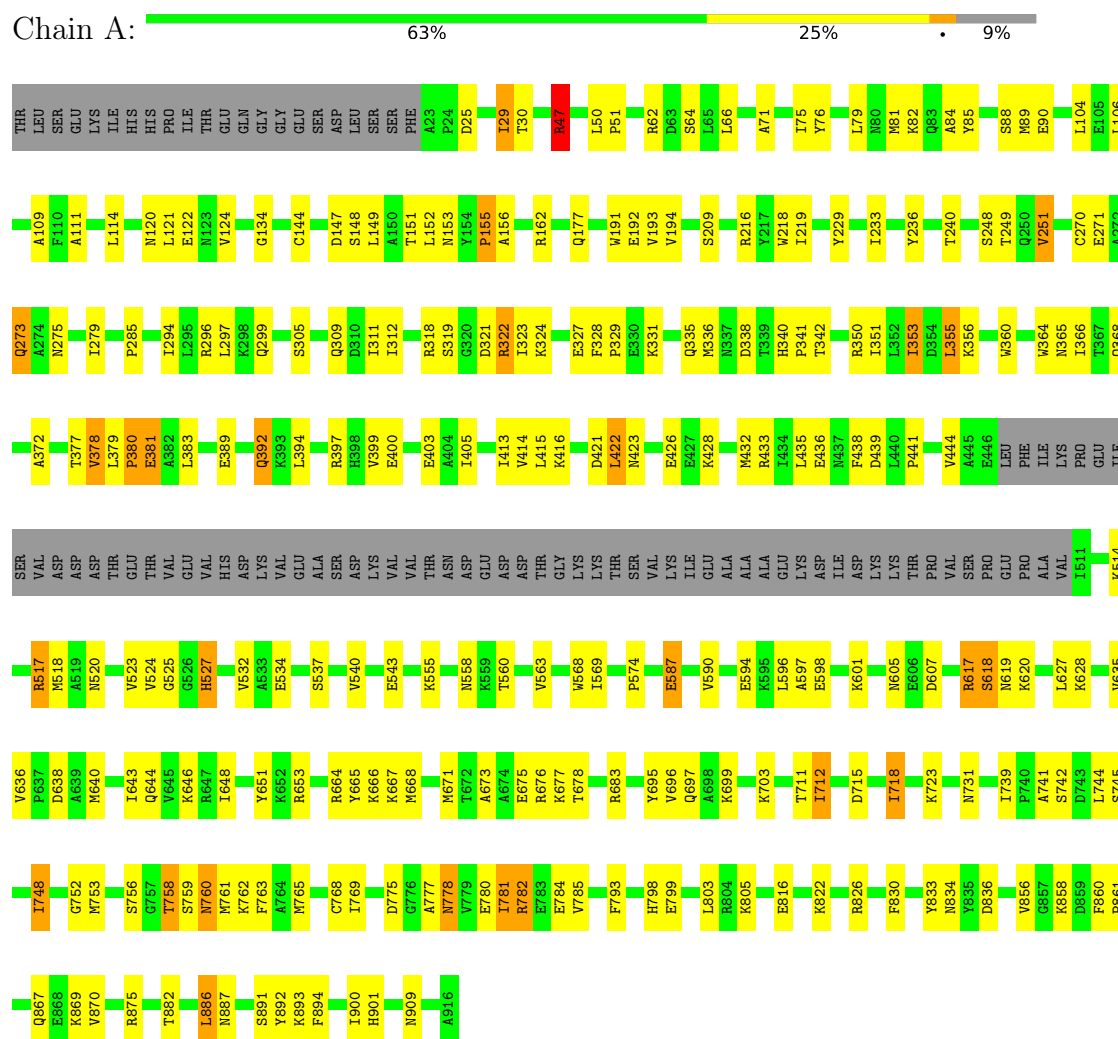
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	C	11	Total	O	0	0
			11	11		

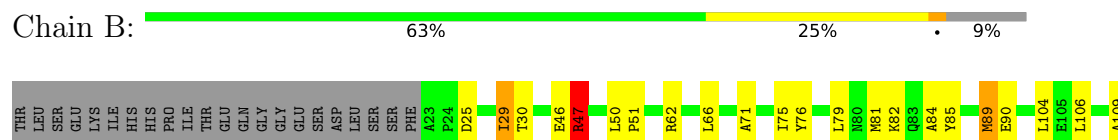
3 Residue-property plots

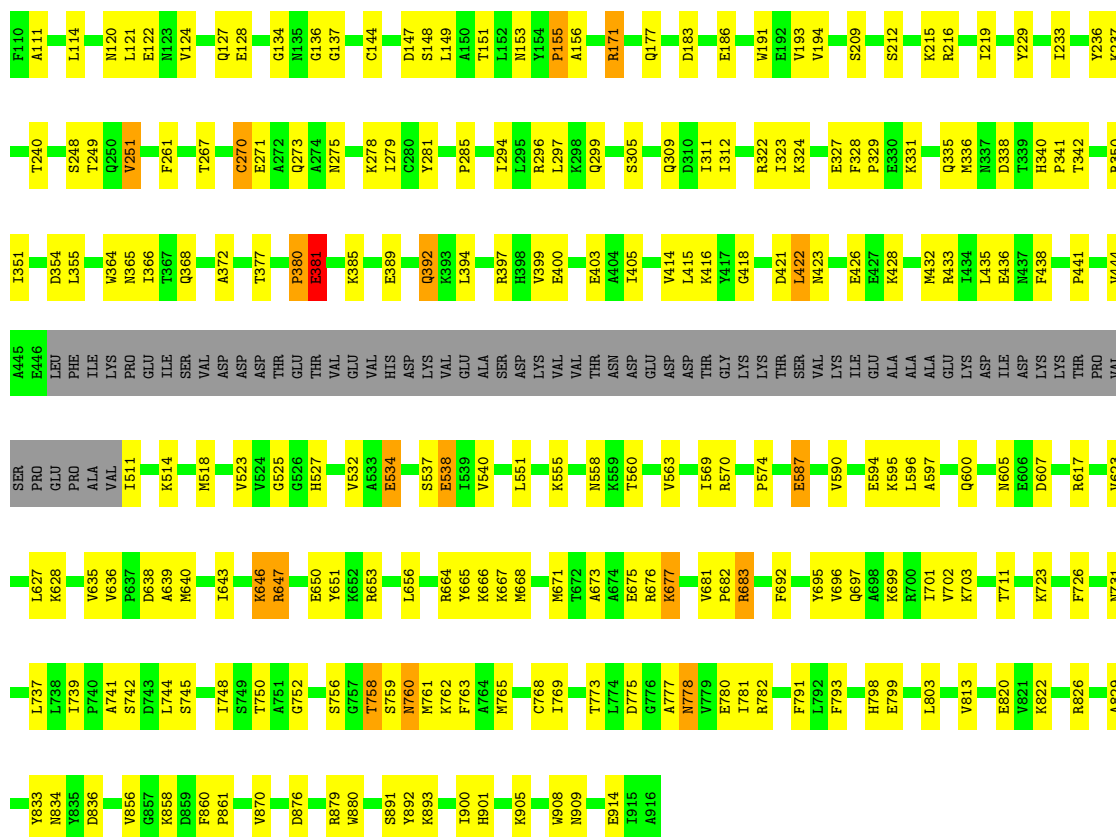
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic



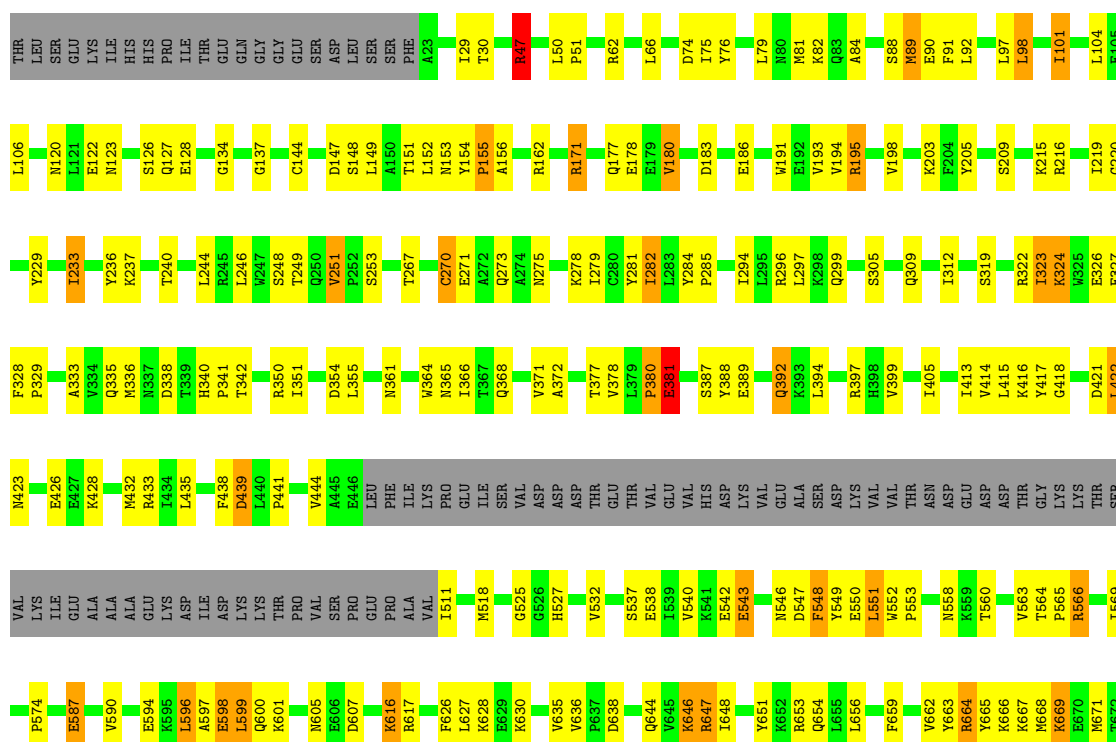
- Molecule 1: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic

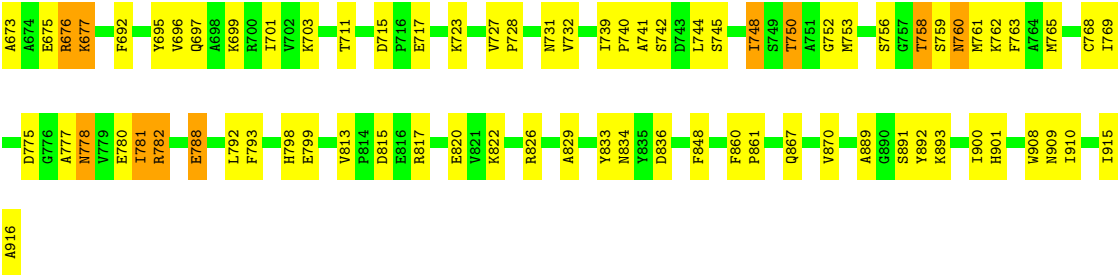




- Molecule 1: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic

Chain C: 59% 27% 9%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.83Å 136.09Å 123.19Å 90.00° 91.55° 90.00°	Depositor
Resolution (Å)	49.54 – 3.70 49.54 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.54-3.70) 90.1 (49.54-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.279 , 0.308 0.294 , 0.322	Depositor DCC
R_{free} test set	1906 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	81.4	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.119 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20042	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, GOL, CFF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/6790	1.07	1/9188 (0.0%)
1	B	0.48	0/6790	1.07	5/9188 (0.1%)
1	C	0.49	0/6790	1.07	1/9188 (0.0%)
All	All	0.49	0/20370	1.07	7/27564 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	PRO	N-CA-C	6.89	119.10	110.70
1	C	574	PRO	N-CA-C	6.82	119.02	110.70
1	A	574	PRO	N-CA-C	6.71	118.88	110.70
1	B	914	GLU	CB-CG-CD	5.70	122.29	112.60
1	B	534	GLU	CB-CG-CD	5.46	121.89	112.60
1	B	538	GLU	CB-CG-CD	5.18	121.40	112.60
1	B	692	PHE	CA-CB-CG	5.08	118.88	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6664	0	6538	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6664	0	6538	151	0
1	C	6664	0	6535	288	0
2	A	12	0	16	1	0
2	C	6	0	8	0	0
3	C	14	0	10	3	0
4	A	7	0	0	0	0
4	C	11	0	0	0	0
All	All	20042	0	19645	631	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (631) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:THR:OG1	1:C:566:ARG:NH2	1.56	1.39
1:C:336:MET:HE1	1:C:371:VAL:CG1	1.56	1.36
1:C:336:MET:CE	1:C:371:VAL:HG13	1.61	1.30
1:C:147:ASP:OD1	1:C:566:ARG:NE	1.70	1.21
1:C:151:THR:CB	1:C:566:ARG:HH22	1.52	1.21
1:A:351:ILE:HG23	1:A:355:LEU:HD11	1.19	1.17
1:C:548:PHE:HA	1:C:551:LEU:HD23	1.28	1.14
1:A:617:ARG:NH1	1:A:638:ASP:OD1	1.82	1.13
1:C:152:LEU:HD11	1:C:154:TYR:CD2	1.83	1.12
1:C:547:ASP:O	1:C:551:LEU:CD2	1.99	1.11
1:C:151:THR:CB	1:C:566:ARG:NH2	2.09	1.10
1:C:548:PHE:HA	1:C:551:LEU:CD2	1.81	1.10
1:C:364:TRP:CZ3	1:C:405:ILE:HG12	1.87	1.09
1:C:364:TRP:HZ3	1:C:405:ILE:HG12	1.00	1.08
1:C:336:MET:HE1	1:C:371:VAL:HG12	1.32	1.07
1:C:669:LYS:HE3	1:C:715:ASP:OD2	1.54	1.07
1:A:319:SER:O	1:A:322:ARG:NE	1.89	1.05
1:C:152:LEU:HD11	1:C:154:TYR:CE2	1.92	1.03
1:C:564:THR:OG1	1:C:566:ARG:CD	2.07	1.02
1:C:547:ASP:O	1:C:551:LEU:HD22	1.57	1.02
1:C:151:THR:HB	1:C:566:ARG:HH22	1.24	1.01
1:B:432:MET:HE1	1:B:551:LEU:HD22	1.40	0.99
1:A:759:SER:N	1:A:762:LLP:H5'1	1.78	0.99
1:A:218:TRP:HE3	1:A:350:ARG:NH1	1.62	0.97
1:C:548:PHE:CA	1:C:551:LEU:CD2	2.44	0.96
1:C:336:MET:CE	1:C:371:VAL:CG1	2.28	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:GLU:N	1:C:546:ASN:HD21	1.63	0.95
1:A:678:THR:O	1:A:875:ARG:NH2	1.99	0.94
1:C:155:PRO:HG2	1:C:910:ILE:HD11	1.49	0.92
1:C:867:GLN:O	1:C:870:VAL:HG22	1.70	0.91
1:C:336:MET:HE2	1:C:371:VAL:HG13	1.50	0.91
1:C:203:LYS:HE3	1:C:220:GLY:O	1.71	0.91
1:C:216:ARG:HH11	1:C:397:ARG:HH11	1.15	0.91
1:A:867:GLN:O	1:A:870:VAL:HG22	1.71	0.90
1:C:92:LEU:HD22	1:C:732:VAL:CG2	2.01	0.90
1:C:335:GLN:HG2	1:C:908:TRP:HE1	1.35	0.90
1:C:171:ARG:NH1	1:C:180:VAL:HG21	1.87	0.90
1:A:351:ILE:CG2	1:A:355:LEU:HD11	2.01	0.90
1:C:659:PHE:HA	1:C:662:VAL:HG22	1.54	0.90
1:C:335:GLN:CG	1:C:908:TRP:HE1	1.84	0.89
1:C:147:ASP:CG	1:C:566:ARG:HE	1.80	0.89
1:C:551:LEU:HD22	1:C:551:LEU:H	1.35	0.88
1:C:564:THR:OG1	1:C:566:ARG:HD3	1.74	0.87
1:C:335:GLN:CD	1:C:908:TRP:NE1	2.32	0.87
1:C:548:PHE:CA	1:C:551:LEU:HD23	2.04	0.87
1:C:547:ASP:O	1:C:551:LEU:HD21	1.71	0.87
1:A:568:TRP:CE2	1:A:762:LLP:HE3	2.10	0.86
1:A:617:ARG:HH11	1:A:638:ASP:CG	1.84	0.86
1:A:568:TRP:CZ2	1:A:762:LLP:HE3	2.11	0.85
1:C:98:LEU:O	1:C:101:ILE:HD13	1.77	0.85
1:A:218:TRP:CE3	1:A:350:ARG:NH1	2.44	0.84
1:B:236:TYR:CE2	1:B:237:LYS:HD3	2.12	0.84
1:A:759:SER:N	1:A:762:LLP:C5'	2.40	0.84
1:A:617:ARG:NH1	1:A:638:ASP:CG	2.36	0.84
1:C:547:ASP:C	1:C:551:LEU:HD21	2.03	0.83
1:C:171:ARG:HG3	1:C:178:GLU:HB2	1.60	0.83
1:C:216:ARG:HH11	1:C:397:ARG:NH1	1.75	0.83
1:A:218:TRP:HE3	1:A:350:ARG:HH11	1.22	0.82
1:A:759:SER:HB3	1:A:762:LLP:H5'1	1.62	0.82
1:C:659:PHE:HA	1:C:662:VAL:CG2	2.09	0.81
1:B:640:MET:SD	1:B:683:ARG:NH1	2.53	0.80
1:A:318:ARG:O	1:A:322:ARG:NH2	2.14	0.80
1:C:335:GLN:NE2	1:C:908:TRP:CD1	2.50	0.80
1:C:782:ARG:HH12	1:C:792:LEU:HD13	1.47	0.79
1:A:640:MET:HG2	1:A:683:ARG:HD3	1.63	0.78
1:A:759:SER:CA	1:A:762:LLP:H5'1	2.13	0.78
1:C:364:TRP:HH2	1:C:405:ILE:HG23	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:THR:OG1	1:C:566:ARG:HD2	1.85	0.77
1:C:92:LEU:CD2	1:C:732:VAL:CG2	2.62	0.77
1:C:319:SER:O	1:C:322:ARG:HG3	1.84	0.77
1:C:782:ARG:HH22	1:C:792:LEU:HB2	1.49	0.77
1:C:782:ARG:HH22	1:C:792:LEU:CB	1.98	0.76
1:C:364:TRP:CH2	1:C:405:ILE:HG23	2.21	0.76
1:B:47:ARG:HB2	1:B:47:ARG:CZ	2.14	0.76
1:C:697:GLN:O	1:C:701:ILE:HD12	1.85	0.76
1:B:261:PHE:HE2	1:C:282:ILE:HD11	1.51	0.76
1:C:92:LEU:HD22	1:C:732:VAL:HG22	1.66	0.75
1:A:759:SER:H	1:A:762:LLP:H5'1	1.50	0.75
1:C:335:GLN:CG	1:C:908:TRP:NE1	2.50	0.74
1:C:364:TRP:HZ3	1:C:405:ILE:CG1	1.91	0.74
1:A:759:SER:CB	1:A:762:LLP:H5'1	2.17	0.74
1:A:882:THR:O	1:A:886:LEU:HD22	1.87	0.74
1:C:368:GLN:HA	1:C:525:GLY:O	1.88	0.74
1:A:368:GLN:HA	1:A:525:GLY:O	1.89	0.73
1:A:671:MET:HG2	1:A:675:GLU:HB2	1.71	0.73
1:C:671:MET:HG2	1:C:675:GLU:HB2	1.71	0.73
1:A:759:SER:H	1:A:762:LLP:C5'	2.02	0.72
1:C:319:SER:O	1:C:322:ARG:CG	2.37	0.72
1:B:368:GLN:HA	1:B:525:GLY:O	1.88	0.72
1:B:671:MET:HG2	1:B:675:GLU:HB2	1.71	0.72
1:A:153:ASN:HA	1:A:240:THR:HG21	1.70	0.72
1:C:563:VAL:HG11	1:C:762:LLP:HE3	1.71	0.72
1:A:351:ILE:O	1:A:355:LEU:HG	1.89	0.71
1:B:153:ASN:HA	1:B:240:THR:HG21	1.70	0.71
1:A:617:ARG:O	1:A:620:LYS:N	2.23	0.71
1:A:436:GLU:CD	1:A:517:ARG:NH2	2.49	0.71
1:C:336:MET:HE3	1:C:372:ALA:O	1.91	0.71
1:C:147:ASP:OD1	1:C:566:ARG:CZ	2.39	0.71
1:A:785:VAL:CG2	1:A:887:ASN:HA	2.21	0.71
1:C:659:PHE:CA	1:C:662:VAL:HG22	2.21	0.71
1:C:153:ASN:HA	1:C:240:THR:HG21	1.71	0.70
1:B:216:ARG:NH2	1:B:400:GLU:CD	2.49	0.70
1:C:547:ASP:C	1:C:551:LEU:CD2	2.64	0.70
1:C:152:LEU:HD12	1:C:152:LEU:O	1.92	0.70
1:A:703:LYS:HE2	1:A:833:TYR:CD2	2.28	0.69
1:B:186:GLU:OE1	1:C:253:SER:OG	2.07	0.69
1:A:785:VAL:HG21	1:A:887:ASN:HA	1.73	0.69
1:C:543:GLU:CA	1:C:546:ASN:HD21	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ARG:HB2	1:C:47:ARG:CZ	2.22	0.69
1:B:703:LYS:HE2	1:B:833:TYR:CD2	2.27	0.68
1:C:703:LYS:HE2	1:C:833:TYR:CD2	2.27	0.68
1:C:548:PHE:HD1	1:C:548:PHE:H	1.40	0.68
1:B:261:PHE:CE2	1:C:282:ILE:HD11	2.27	0.68
1:A:643:ILE:HD12	1:A:742:SER:HB3	1.76	0.67
1:C:335:GLN:HG2	1:C:908:TRP:NE1	2.05	0.67
1:B:364:TRP:CZ3	1:B:405:ILE:HG12	2.30	0.67
1:C:653:ARG:NH1	1:C:750:THR:HA	2.10	0.67
1:C:564:THR:HG1	1:C:566:ARG:CD	2.06	0.67
1:A:711:THR:HG21	1:A:830:PHE:HA	1.77	0.67
1:B:563:VAL:HG11	1:B:762:LLP:HE3	1.77	0.67
1:A:640:MET:CG	1:A:683:ARG:HD3	2.26	0.66
1:A:784:GLU:OE1	1:A:893:LYS:NZ	2.24	0.66
1:C:692:PHE:CD1	3:C:1002:CFF:C14	2.79	0.66
1:B:340:HIS:HB2	1:B:341:PRO:HD3	1.78	0.66
1:B:537:SER:O	1:B:540:VAL:HG22	1.96	0.66
1:C:548:PHE:HA	1:C:551:LEU:HD21	1.74	0.66
1:C:216:ARG:NH1	1:C:397:ARG:HH11	1.92	0.66
1:A:340:HIS:HB2	1:A:341:PRO:HD3	1.76	0.66
1:B:643:ILE:HD12	1:B:742:SER:HB3	1.78	0.66
1:C:91:PHE:CE2	1:C:244:LEU:HD11	2.31	0.66
1:B:89:MET:HE1	1:B:299:GLN:HB3	1.78	0.65
1:C:340:HIS:HB2	1:C:341:PRO:HD3	1.78	0.65
1:A:364:TRP:CZ3	1:A:405:ILE:HG12	2.30	0.65
1:C:312:ILE:HD13	1:C:351:ILE:HG21	1.78	0.65
1:B:428:LYS:O	1:B:432:MET:HG3	1.95	0.65
1:C:560:THR:HG21	1:C:780:GLU:OE1	1.98	0.64
1:A:216:ARG:NH2	1:A:400:GLU:CD	2.55	0.64
1:A:273:GLN:HE21	1:A:273:GLN:H	1.46	0.64
1:A:436:GLU:CD	1:A:517:ARG:HH21	2.06	0.64
1:B:656:LEU:HD23	1:B:748:ILE:HD12	1.78	0.64
1:C:324:LYS:HD2	1:C:326:GLU:H	1.63	0.64
1:A:644:GLN:NE2	1:A:748:ILE:CD1	2.62	0.63
1:B:666:LYS:HE2	1:B:820:GLU:HG2	1.80	0.63
1:A:537:SER:O	1:A:540:VAL:HG22	1.99	0.63
1:C:659:PHE:O	1:C:662:VAL:CG2	2.46	0.63
1:A:312:ILE:HD13	1:A:351:ILE:HG21	1.81	0.62
1:A:319:SER:O	1:A:322:ARG:CZ	2.46	0.62
1:C:91:PHE:CD2	1:C:244:LEU:HD11	2.34	0.62
1:A:781:ILE:O	1:A:785:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:644:GLN:NE2	1:C:748:ILE:CD1	2.63	0.62
1:C:548:PHE:C	1:C:551:LEU:CD2	2.73	0.62
1:A:378:VAL:HG21	1:A:753:MET:O	1.99	0.62
1:A:389:GLU:CD	1:A:389:GLU:H	2.08	0.61
1:C:782:ARG:NH2	1:C:792:LEU:HB2	2.15	0.61
1:B:876:ASP:CG	1:B:879:ARG:HB2	2.25	0.61
1:C:342:THR:HB	1:C:518:MET:HE3	1.82	0.61
1:C:542:GLU:C	1:C:546:ASN:HD21	2.08	0.61
1:C:380:PRO:O	1:C:381:GLU:HB3	2.01	0.61
1:B:711:THR:HG21	1:B:829:ALA:O	2.00	0.61
1:C:98:LEU:HD23	1:C:101:ILE:CD1	2.31	0.61
1:A:368:GLN:O	1:A:527:HIS:HB3	2.01	0.61
1:B:312:ILE:HD13	1:B:351:ILE:HG21	1.83	0.61
1:C:152:LEU:HD11	1:C:154:TYR:CG	2.34	0.60
1:C:368:GLN:O	1:C:527:HIS:HB3	2.01	0.60
1:B:389:GLU:H	1:B:389:GLU:CD	2.09	0.60
1:A:355:LEU:CD1	1:A:356:LYS:HE2	2.32	0.60
1:B:380:PRO:O	1:B:381:GLU:HB3	2.01	0.60
1:C:282:ILE:HD12	1:C:282:ILE:H	1.66	0.60
1:C:548:PHE:CA	1:C:551:LEU:HD21	2.29	0.60
1:C:744:LEU:HA	1:C:769:ILE:O	2.02	0.60
1:B:744:LEU:HA	1:B:769:ILE:O	2.02	0.59
1:A:380:PRO:O	1:A:381:GLU:HB3	2.01	0.59
1:C:98:LEU:HD23	1:C:101:ILE:HD11	1.83	0.59
1:B:773:THR:O	1:B:778:ASN:ND2	2.27	0.59
1:C:428:LYS:O	1:C:432:MET:HG3	2.02	0.59
1:C:659:PHE:O	1:C:662:VAL:HG23	2.01	0.59
1:B:215:LYS:HE3	1:B:354:ASP:O	2.02	0.59
1:B:90:GLU:HB2	1:B:134:GLY:HA2	1.84	0.59
1:B:368:GLN:O	1:B:527:HIS:HB3	2.03	0.59
1:C:669:LYS:HE2	1:C:717:GLU:OE1	2.03	0.59
1:A:644:GLN:NE2	1:A:748:ILE:HD11	2.17	0.59
1:C:177:GLN:HE21	1:C:699:LYS:HE3	1.68	0.58
1:A:324:LYS:O	1:A:327:GLU:HB2	2.03	0.58
1:C:324:LYS:O	1:C:327:GLU:HB2	2.03	0.58
1:B:594:GLU:HA	1:B:892:TYR:CD2	2.39	0.58
1:C:617:ARG:NH1	1:C:638:ASP:OD1	2.37	0.58
1:A:892:TYR:CZ	1:A:893:LYS:HE3	2.39	0.58
1:A:640:MET:SD	1:A:683:ARG:HD3	2.43	0.58
1:A:643:ILE:CD1	1:A:742:SER:HB3	2.34	0.58
1:A:744:LEU:HA	1:A:769:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:HD12	1:A:356:LYS:CD	2.33	0.58
1:A:413:ILE:CD1	1:A:432:MET:HE3	2.34	0.58
1:A:380:PRO:HA	1:A:383:LEU:HD23	1.86	0.58
1:B:177:GLN:HE21	1:B:699:LYS:HE3	1.68	0.58
1:C:711:THR:HG21	1:C:829:ALA:O	2.03	0.57
1:C:775:ASP:O	1:C:778:ASN:HB2	2.04	0.57
1:A:350:ARG:HD2	1:A:397:ARG:HG2	1.86	0.57
1:A:617:ARG:NH1	1:A:638:ASP:OD2	2.37	0.57
1:A:617:ARG:O	1:A:618:SER:C	2.47	0.57
1:C:236:TYR:CE2	1:C:237:LYS:HG3	2.39	0.57
1:C:90:GLU:HB2	1:C:134:GLY:HA2	1.85	0.57
1:A:594:GLU:HA	1:A:892:TYR:CD2	2.39	0.57
1:A:177:GLN:HE21	1:A:699:LYS:HE3	1.69	0.57
1:A:568:TRP:CH2	1:A:762:LLP:HE3	2.40	0.57
1:A:775:ASP:O	1:A:778:ASN:HB2	2.05	0.57
1:A:803:LEU:HD22	1:A:858:LYS:HE3	1.85	0.57
1:A:891:SER:O	1:A:894:PHE:HD1	1.86	0.57
1:C:89:MET:CE	1:C:299:GLN:HB3	2.34	0.57
1:C:413:ILE:CD1	1:C:432:MET:HE3	2.34	0.57
1:A:711:THR:OG1	1:A:830:PHE:HD1	1.88	0.56
1:B:392:GLN:HA	1:B:399:VAL:HG21	1.87	0.56
1:C:203:LYS:CE	1:C:220:GLY:O	2.48	0.56
1:C:594:GLU:HA	1:C:892:TYR:CD2	2.39	0.56
1:A:120:ASN:HD21	1:A:122:GLU:HG2	1.70	0.56
1:B:681:VAL:HG23	1:B:683:ARG:HD3	1.87	0.56
1:B:775:ASP:O	1:B:778:ASN:HB2	2.06	0.56
1:A:392:GLN:HA	1:A:399:VAL:HG21	1.87	0.56
1:C:644:GLN:NE2	1:C:748:ILE:HD11	2.20	0.56
1:B:860:PHE:HB3	1:B:861:PRO:HD3	1.87	0.56
1:A:752:GLY:H	1:A:775:ASP:CB	2.19	0.56
1:B:569:ILE:HD11	1:B:765:MET:HB3	1.87	0.55
1:A:667:LYS:O	1:A:671:MET:HE3	2.07	0.55
1:A:29:ILE:HD13	1:A:109:ALA:HB1	1.89	0.55
1:B:643:ILE:CD1	1:B:742:SER:HB3	2.36	0.55
1:B:791:PHE:CZ	1:B:870:VAL:HA	2.41	0.55
1:C:692:PHE:CD1	3:C:1002:CFF:H141	2.40	0.55
1:A:762:LLP:P	1:A:762:LLP:H6	2.47	0.55
1:B:120:ASN:HD21	1:B:122:GLU:HG2	1.71	0.55
1:C:324:LYS:HG3	1:C:326:GLU:HB3	1.89	0.55
1:C:667:LYS:O	1:C:671:MET:HE3	2.05	0.55
1:C:860:PHE:HB3	1:C:861:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB2	1:A:134:GLY:HA2	1.89	0.55
1:A:335:GLN:OE1	1:A:372:ALA:HB3	2.06	0.55
1:B:335:GLN:OE1	1:B:372:ALA:HB3	2.07	0.55
1:B:671:MET:HG2	1:B:675:GLU:CB	2.37	0.55
1:B:216:ARG:HH21	1:B:400:GLU:CD	2.15	0.54
1:C:97:LEU:O	1:C:101:ILE:HG23	2.07	0.54
1:C:335:GLN:CD	1:C:908:TRP:CD1	2.84	0.54
1:C:251:VAL:HG12	1:C:273:GLN:HB3	1.89	0.54
1:C:548:PHE:CD1	1:C:548:PHE:N	2.71	0.54
1:A:860:PHE:HB3	1:A:861:PRO:HD3	1.88	0.54
1:A:671:MET:HG2	1:A:675:GLU:CB	2.37	0.54
1:A:762:LLP:O	1:A:765:MET:N	2.41	0.54
1:A:745:SER:HB3	1:A:768:CYS:SG	2.47	0.54
1:C:668:MET:O	1:C:676:ARG:HD3	2.08	0.54
1:C:762:LLP:O	1:C:765:MET:N	2.41	0.54
1:A:329:PRO:HG3	1:A:366:ILE:HG23	1.88	0.54
1:A:355:LEU:HD12	1:A:356:LYS:HD3	1.89	0.54
1:A:777:ALA:O	1:A:781:ILE:HG13	2.08	0.54
1:B:667:LYS:O	1:B:671:MET:HE3	2.08	0.54
1:C:151:THR:CG2	1:C:566:ARG:HH22	2.19	0.54
1:B:50:LEU:HB2	1:B:51:PRO:HD3	1.88	0.53
1:B:803:LEU:HD22	1:B:858:LYS:HE3	1.90	0.53
1:C:537:SER:O	1:C:540:VAL:HG12	2.08	0.53
1:C:543:GLU:N	1:C:546:ASN:ND2	2.46	0.53
1:C:564:THR:HG1	1:C:566:ARG:HD2	1.72	0.53
1:C:692:PHE:CD1	3:C:1002:CFF:H143	2.41	0.53
1:C:778:ASN:HA	1:C:781:ILE:HD11	1.90	0.53
1:A:678:THR:C	1:A:875:ARG:HH22	2.14	0.53
1:C:435:LEU:HB3	1:C:438:PHE:CD2	2.44	0.53
1:A:569:ILE:HD11	1:A:765:MET:HB3	1.90	0.53
1:B:762:LLP:O	1:B:765:MET:N	2.41	0.53
1:C:82:LYS:HD3	1:C:909:ASN:O	2.08	0.53
1:C:205:TYR:CE1	1:C:394:LEU:HD12	2.43	0.53
1:C:548:PHE:C	1:C:551:LEU:HD23	2.34	0.53
1:C:671:MET:HG2	1:C:675:GLU:CB	2.38	0.53
1:A:216:ARG:HH21	1:A:400:GLU:CD	2.17	0.53
1:B:745:SER:HB3	1:B:768:CYS:SG	2.49	0.53
1:C:731:ASN:C	1:C:731:ASN:OD1	2.52	0.53
1:B:329:PRO:HG3	1:B:366:ILE:HG23	1.90	0.53
1:C:392:GLN:HA	1:C:399:VAL:HG21	1.90	0.53
1:A:111:ALA:HB2	1:A:121:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:LYS:O	1:C:826:ARG:HG3	2.09	0.53
1:C:137:GLY:CA	1:C:762:LLP:H5'2	2.39	0.53
1:C:171:ARG:NH1	1:C:180:VAL:CG2	2.68	0.53
1:B:82:LYS:HD3	1:B:909:ASN:O	2.09	0.52
1:B:89:MET:CE	1:B:299:GLN:HB3	2.38	0.52
1:C:569:ILE:HD11	1:C:765:MET:HB3	1.91	0.52
1:A:355:LEU:HD12	1:A:356:LYS:HG2	1.90	0.52
1:B:183:ASP:O	1:B:186:GLU:HB2	2.09	0.52
1:C:76:TYR:CE2	1:C:155:PRO:HA	2.44	0.52
1:C:120:ASN:HD21	1:C:122:GLU:HG2	1.74	0.52
1:C:152:LEU:CD1	1:C:154:TYR:CE2	2.80	0.52
1:A:673:ALA:O	1:A:677:LYS:HD2	2.08	0.52
1:C:745:SER:HB3	1:C:768:CYS:SG	2.48	0.52
1:A:82:LYS:HD3	1:A:909:ASN:O	2.08	0.52
1:B:76:TYR:CE2	1:B:155:PRO:HA	2.45	0.52
1:B:216:ARG:NH2	1:B:400:GLU:OE1	2.42	0.52
1:B:731:ASN:OD1	1:B:731:ASN:C	2.52	0.52
1:A:617:ARG:O	1:A:619:ASN:N	2.42	0.52
1:A:731:ASN:C	1:A:731:ASN:OD1	2.52	0.52
1:B:111:ALA:HB2	1:B:121:LEU:HD22	1.92	0.52
1:B:351:ILE:HA	1:B:355:LEU:HD12	1.91	0.52
1:B:635:VAL:HG12	1:B:723:LYS:HG3	1.92	0.52
1:C:329:PRO:HG3	1:C:366:ILE:HG23	1.91	0.52
1:B:650:GLU:OE2	1:B:697:GLN:HG2	2.10	0.52
1:B:681:VAL:CG2	1:B:683:ARG:HD3	2.40	0.52
1:A:76:TYR:CE2	1:A:155:PRO:HA	2.45	0.51
1:A:104:LEU:HB3	1:A:106:LEU:HD12	1.91	0.51
1:A:644:GLN:HE22	1:A:748:ILE:HD11	1.75	0.51
1:C:123:ASN:O	1:C:126:SER:OG	2.21	0.51
1:C:659:PHE:C	1:C:662:VAL:HG22	2.34	0.51
1:B:433:ARG:HH22	1:B:438:PHE:HB3	1.76	0.51
1:C:236:TYR:OH	1:C:237:LYS:HE3	2.10	0.51
1:A:635:VAL:HG12	1:A:723:LYS:HG3	1.92	0.51
1:C:653:ARG:HH21	1:C:656:LEU:HD22	1.75	0.51
1:A:534:GLU:HG2	1:A:780:GLU:OE2	2.11	0.51
1:A:785:VAL:HG23	1:A:887:ASN:HA	1.92	0.51
1:A:597:ALA:HB2	1:A:892:TYR:CE1	2.46	0.51
1:C:294:ILE:HG23	1:C:394:LEU:HD13	1.93	0.51
1:C:777:ALA:O	1:C:781:ILE:HG12	2.10	0.51
1:A:568:TRP:CD2	1:A:762:LLP:HE3	2.45	0.51
1:A:748:ILE:HD13	1:A:748:ILE:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:GLY:H	1:B:775:ASP:CB	2.22	0.51
1:C:155:PRO:HG2	1:C:910:ILE:CD1	2.32	0.50
1:C:752:GLY:H	1:C:775:ASP:CB	2.23	0.50
1:B:822:LYS:O	1:B:826:ARG:HG3	2.11	0.50
1:A:739:ILE:C	1:A:741:ALA:H	2.20	0.50
1:C:155:PRO:CG	1:C:910:ILE:HD11	2.32	0.50
1:A:328:PHE:HB3	1:A:329:PRO:HD3	1.93	0.50
1:C:653:ARG:HH11	1:C:750:THR:HA	1.75	0.50
1:C:673:ALA:O	1:C:677:LYS:HD2	2.12	0.50
1:A:568:TRP:CZ2	1:A:762:LLP:CE	2.91	0.50
1:C:761:MET:O	1:C:765:MET:HG3	2.12	0.50
1:B:328:PHE:HB3	1:B:329:PRO:HD3	1.94	0.50
1:C:147:ASP:OD1	1:C:566:ARG:NH2	2.45	0.50
1:C:665:TYR:O	1:C:668:MET:HB2	2.12	0.50
1:A:392:GLN:HG2	1:A:399:VAL:HG11	1.93	0.50
1:B:617:ARG:NH1	1:B:638:ASP:OD1	2.45	0.50
1:A:433:ARG:HH22	1:A:438:PHE:HB3	1.77	0.49
1:B:673:ALA:O	1:B:677:LYS:HD2	2.12	0.49
1:C:328:PHE:HB3	1:C:329:PRO:HD3	1.94	0.49
1:C:104:LEU:HB3	1:C:106:LEU:HD12	1.93	0.49
1:C:151:THR:CG2	1:C:566:ARG:NH2	2.72	0.49
1:C:413:ILE:HD11	1:C:432:MET:HE3	1.94	0.49
1:C:659:PHE:O	1:C:662:VAL:HG22	2.11	0.49
1:B:104:LEU:HB3	1:B:106:LEU:HD12	1.93	0.49
1:C:236:TYR:CZ	1:C:237:LYS:HE3	2.47	0.49
1:B:739:ILE:C	1:B:741:ALA:H	2.20	0.49
1:C:597:ALA:HB2	1:C:892:TYR:CE1	2.47	0.49
1:C:644:GLN:HE22	1:C:748:ILE:HD11	1.77	0.49
1:A:50:LEU:HB2	1:A:51:PRO:HD3	1.94	0.49
1:C:171:ARG:HG3	1:C:178:GLU:CB	2.39	0.49
1:C:566:ARG:CD	1:C:566:ARG:H	2.25	0.49
1:A:294:ILE:HG23	1:A:394:LEU:HD13	1.95	0.49
1:A:900:ILE:O	1:A:901:HIS:C	2.55	0.49
1:B:342:THR:HB	1:B:518:MET:HE3	1.94	0.49
1:C:155:PRO:O	1:C:910:ILE:CD1	2.61	0.49
1:A:25:ASP:O	1:A:29:ILE:HD12	2.13	0.49
1:A:47:ARG:HB2	1:A:47:ARG:CZ	2.35	0.49
1:A:523:VAL:O	1:A:555:LYS:NZ	2.45	0.49
1:B:392:GLN:HG2	1:B:399:VAL:HG11	1.94	0.49
1:A:89:MET:HG3	1:A:340:HIS:HB3	1.95	0.49
1:C:92:LEU:CD2	1:C:732:VAL:HG23	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:HD2	1:C:397:ARG:HG2	1.94	0.48
1:A:353:ILE:HD11	1:A:360:TRP:HA	1.94	0.48
1:C:144:CYS:O	1:C:147:ASP:HB3	2.13	0.48
1:B:249:THR:HG21	1:B:279:ILE:HG21	1.95	0.48
1:C:89:MET:HE3	1:C:299:GLN:HB3	1.94	0.48
1:C:616:LYS:HE2	1:C:741:ALA:HA	1.94	0.48
1:B:294:ILE:HG23	1:B:394:LEU:HD13	1.95	0.48
1:B:900:ILE:O	1:B:901:HIS:C	2.55	0.48
1:C:548:PHE:N	1:C:551:LEU:HD21	2.27	0.48
1:C:663:TYR:CE2	1:C:817:ARG:HB3	2.48	0.48
1:B:25:ASP:O	1:B:29:ILE:HD12	2.14	0.48
1:C:171:ARG:HH12	1:C:180:VAL:HG21	1.73	0.48
1:C:653:ARG:HD3	1:C:750:THR:OG1	2.14	0.48
1:C:867:GLN:O	1:C:870:VAL:CG2	2.54	0.48
1:A:665:TYR:O	1:A:668:MET:HB2	2.14	0.48
1:B:653:ARG:HG2	1:B:856:VAL:HG22	1.95	0.48
1:C:428:LYS:NZ	1:C:550:GLU:OE2	2.45	0.48
1:B:336:MET:HG2	1:B:341:PRO:HB2	1.95	0.48
1:B:597:ALA:HB2	1:B:892:TYR:CE1	2.49	0.48
1:C:739:ILE:C	1:C:741:ALA:H	2.21	0.48
1:A:249:THR:HG21	1:A:279:ILE:HG21	1.96	0.47
1:A:822:LYS:O	1:A:826:ARG:HG3	2.13	0.47
1:B:681:VAL:O	1:B:683:ARG:HG2	2.14	0.47
1:C:50:LEU:HB2	1:C:51:PRO:HD3	1.95	0.47
1:C:900:ILE:O	1:C:901:HIS:C	2.56	0.47
1:C:151:THR:HG21	1:C:566:ARG:NH1	2.29	0.47
1:C:249:THR:HG21	1:C:279:ILE:HG21	1.96	0.47
1:B:364:TRP:O	1:B:368:GLN:HG3	2.15	0.47
1:A:251:VAL:CG1	1:A:273:GLN:HB3	2.44	0.47
1:A:355:LEU:HD12	1:A:356:LYS:CG	2.44	0.47
1:B:665:TYR:O	1:B:668:MET:HB2	2.14	0.47
1:C:635:VAL:HG12	1:C:723:LYS:HG3	1.96	0.47
1:C:336:MET:SD	1:C:371:VAL:HG13	2.51	0.47
1:A:527:HIS:CE1	2:A:1101:GOL:O2	2.67	0.47
1:C:84:ALA:O	1:C:156:ALA:HA	2.15	0.47
1:C:296:ARG:O	1:C:299:GLN:HB2	2.14	0.47
1:C:596:LEU:O	1:C:599:LEU:HG	2.14	0.47
1:C:351:ILE:HA	1:C:355:LEU:HD12	1.96	0.47
1:A:653:ARG:HG2	1:A:856:VAL:HG22	1.97	0.47
1:C:216:ARG:NH1	1:C:397:ARG:NH1	2.55	0.47
1:C:285:PRO:HD3	1:C:299:GLN:HE22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:GLN:HG2	1:C:399:VAL:HG11	1.96	0.47
1:A:251:VAL:HG12	1:A:273:GLN:HB3	1.97	0.47
1:A:342:THR:HB	1:A:518:MET:HE3	1.97	0.47
1:A:364:TRP:O	1:A:368:GLN:HG3	2.15	0.47
1:C:666:LYS:NZ	1:C:820:GLU:HG2	2.30	0.47
1:C:364:TRP:O	1:C:368:GLN:HG3	2.14	0.47
1:C:433:ARG:HH22	1:C:438:PHE:HB3	1.79	0.47
1:A:148:SER:O	1:A:151:THR:N	2.49	0.46
1:A:781:ILE:O	1:A:782:ARG:C	2.58	0.46
1:C:551:LEU:CD2	1:C:551:LEU:H	2.18	0.46
1:A:144:CYS:O	1:A:147:ASP:HB3	2.15	0.46
1:B:296:ARG:O	1:B:299:GLN:HB2	2.15	0.46
1:B:532:VAL:O	1:B:560:THR:HA	2.16	0.46
1:C:598:GLU:HG3	1:C:601:LYS:NZ	2.29	0.46
1:A:762:LLP:O	1:A:763:PHE:C	2.59	0.46
1:B:194:VAL:HG22	1:B:229:TYR:CD2	2.51	0.46
1:B:761:MET:O	1:B:765:MET:HG3	2.15	0.46
1:C:697:GLN:C	1:C:701:ILE:HD12	2.38	0.46
1:A:665:TYR:CD1	1:A:712:ILE:HD13	2.51	0.46
1:A:761:MET:O	1:A:765:MET:HG3	2.16	0.46
1:C:336:MET:HG2	1:C:341:PRO:HB2	1.98	0.46
1:C:551:LEU:HD22	1:C:551:LEU:N	2.16	0.46
1:C:627:LEU:O	1:C:628:LYS:C	2.59	0.46
1:B:148:SER:O	1:B:151:THR:N	2.49	0.46
1:C:417:TYR:OH	1:C:551:LEU:CD1	2.63	0.46
1:C:215:LYS:HD2	1:C:354:ASP:O	2.16	0.46
1:C:251:VAL:CG1	1:C:273:GLN:HB3	2.46	0.46
1:C:439:ASP:OD1	1:C:439:ASP:N	2.45	0.46
1:A:759:SER:N	1:A:762:LLP:H5'2	2.29	0.46
1:B:627:LEU:O	1:B:628:LYS:C	2.58	0.46
1:C:183:ASP:O	1:C:186:GLU:HB2	2.15	0.46
1:B:66:LEU:HD21	1:B:193:VAL:HG21	1.98	0.46
1:B:144:CYS:O	1:B:147:ASP:HB3	2.16	0.46
1:A:403:GLU:HG2	1:A:435:LEU:HD11	1.98	0.45
1:A:627:LEU:O	1:A:628:LYS:C	2.59	0.45
1:B:534:GLU:O	1:B:538:GLU:HG2	2.16	0.45
1:C:792:LEU:HG	1:C:793:PHE:N	2.31	0.45
1:A:84:ALA:O	1:A:156:ALA:HA	2.16	0.45
1:C:194:VAL:HG22	1:C:229:TYR:CD2	2.52	0.45
1:A:285:PRO:HD3	1:A:299:GLN:HE22	1.82	0.45
1:A:338:ASP:O	1:A:341:PRO:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ALA:O	1:B:156:ALA:HA	2.17	0.45
1:C:543:GLU:CA	1:C:546:ASN:ND2	2.78	0.45
1:C:781:ILE:O	1:C:782:ARG:C	2.59	0.45
1:A:305:SER:O	1:A:309:GLN:HG3	2.17	0.45
1:C:171:ARG:HH11	1:C:180:VAL:HG21	1.74	0.45
1:C:338:ASP:O	1:C:341:PRO:HD2	2.17	0.45
1:C:762:LLP:O	1:C:763:PHE:C	2.59	0.45
1:A:296:ARG:O	1:A:299:GLN:HB2	2.17	0.45
1:A:532:VAL:O	1:A:560:THR:HA	2.15	0.45
1:C:148:SER:O	1:C:151:THR:N	2.50	0.45
1:C:319:SER:O	1:C:322:ARG:HG2	2.15	0.45
1:A:114:LEU:HD22	1:A:124:VAL:HG21	1.99	0.45
1:B:664:ARG:O	1:B:668:MET:HG3	2.17	0.45
1:B:338:ASP:O	1:B:341:PRO:HD2	2.16	0.45
1:C:532:VAL:O	1:C:560:THR:HA	2.16	0.45
1:C:537:SER:CB	1:C:558:ASN:HB2	2.47	0.45
1:C:587:GLU:O	1:C:590:VAL:HG23	2.17	0.45
1:B:251:VAL:HG12	1:B:273:GLN:HB3	1.99	0.45
1:B:285:PRO:HD3	1:B:299:GLN:HE22	1.80	0.45
1:B:350:ARG:HD2	1:B:397:ARG:HG2	1.98	0.45
1:C:548:PHE:C	1:C:551:LEU:HD22	2.42	0.45
1:A:194:VAL:HG22	1:A:229:TYR:CD2	2.52	0.45
1:C:759:SER:O	1:C:762:LLP:HG2	2.17	0.44
1:A:617:ARG:CZ	1:A:638:ASP:OD1	2.59	0.44
1:B:62:ARG:HD2	1:B:191:TRP:O	2.17	0.44
1:C:664:ARG:O	1:C:668:MET:HG3	2.17	0.44
1:C:748:ILE:HD13	1:C:748:ILE:H	1.81	0.44
1:A:834:ASN:HD21	1:A:836:ASP:HB2	1.81	0.44
1:B:798:HIS:CE1	1:B:799:GLU:HG3	2.52	0.44
1:C:324:LYS:HA	1:C:324:LYS:HD3	1.77	0.44
1:B:340:HIS:C	1:B:342:THR:H	2.26	0.44
1:C:626:PHE:CE1	1:C:630:LYS:HG3	2.53	0.44
1:A:151:THR:HG23	1:A:236:TYR:HB3	1.99	0.44
1:A:760:ASN:OD1	1:A:760:ASN:N	2.49	0.44
1:B:89:MET:HG2	1:B:340:HIS:HB3	2.00	0.44
1:B:416:LYS:O	1:B:418:GLY:N	2.45	0.44
1:B:758:THR:C	1:B:762:LLP:HE2	2.42	0.44
1:C:548:PHE:O	1:C:551:LEU:HD23	2.17	0.44
1:B:421:ASP:O	1:B:422:LEU:HB2	2.18	0.44
1:C:387:SER:O	1:C:389:GLU:N	2.51	0.44
1:A:89:MET:HG3	1:A:340:HIS:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:VAL:CG1	1:B:273:GLN:HB3	2.48	0.44
1:B:891:SER:O	1:B:893:LYS:N	2.51	0.44
1:B:762:LLP:O	1:B:763:PHE:C	2.60	0.44
1:B:781:ILE:O	1:B:782:ARG:C	2.59	0.44
1:C:88:SER:OG	1:C:90:GLU:O	2.35	0.44
1:C:758:THR:C	1:C:762:LLP:HE2	2.43	0.44
1:C:834:ASN:HD21	1:C:836:ASP:HB2	1.82	0.44
1:A:428:LYS:O	1:A:432:MET:HG3	2.18	0.44
1:A:882:THR:HG22	1:A:886:LEU:CD2	2.48	0.44
1:A:718:ILE:CD1	1:A:718:ILE:N	2.81	0.43
1:B:151:THR:HG23	1:B:236:TYR:HB3	2.00	0.43
1:C:340:HIS:C	1:C:342:THR:H	2.26	0.43
1:C:798:HIS:CE1	1:C:799:GLU:HG3	2.54	0.43
1:C:815:ASP:HB2	1:C:861:PRO:HG3	2.00	0.43
1:A:891:SER:O	1:A:893:LYS:N	2.51	0.43
1:C:727:VAL:HA	1:C:728:PRO:HD3	1.85	0.43
1:A:66:LEU:HD21	1:A:193:VAL:HG21	1.98	0.43
1:A:355:LEU:CD1	1:A:356:LYS:CE	2.96	0.43
1:A:537:SER:CB	1:A:558:ASN:HB2	2.49	0.43
1:A:421:ASP:O	1:A:422:LEU:HB2	2.18	0.43
1:A:665:TYR:O	1:A:666:LYS:C	2.62	0.43
1:A:777:ALA:O	1:A:780:GLU:N	2.51	0.43
1:B:596:LEU:HB2	1:B:892:TYR:HB3	2.00	0.43
1:A:777:ALA:O	1:A:778:ASN:C	2.61	0.43
1:C:152:LEU:HD12	1:C:152:LEU:C	2.43	0.43
1:C:171:ARG:HE	1:C:171:ARG:HB3	1.70	0.43
1:A:748:ILE:HB	1:A:793:PHE:HZ	1.83	0.43
1:B:646:LYS:O	1:B:647:ARG:C	2.61	0.43
1:A:148:SER:O	1:A:149:LEU:C	2.62	0.43
1:B:834:ASN:HD21	1:B:836:ASP:HB2	1.82	0.43
1:C:66:LEU:HD21	1:C:193:VAL:HG21	2.00	0.43
1:C:665:TYR:O	1:C:666:LYS:C	2.61	0.43
1:A:88:SER:OG	1:A:90:GLU:O	2.37	0.43
1:A:336:MET:HG2	1:A:341:PRO:HB2	2.00	0.43
1:A:587:GLU:O	1:A:590:VAL:HG23	2.19	0.43
1:B:114:LEU:HD22	1:B:124:VAL:HG21	2.00	0.43
1:A:114:LEU:HD13	1:A:124:VAL:HG21	2.01	0.42
1:A:364:TRP:CH2	1:A:405:ILE:HG23	2.54	0.42
1:A:563:VAL:HG21	1:A:762:LLP:HG2	2.00	0.42
1:A:664:ARG:O	1:A:668:MET:HG3	2.19	0.42
1:C:758:THR:OG1	1:C:762:LLP:H5'1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:GLN:O	1:A:870:VAL:CG2	2.56	0.42
1:B:71:ALA:O	1:B:75:ILE:HG12	2.19	0.42
1:C:416:LYS:O	1:C:418:GLY:N	2.46	0.42
1:A:340:HIS:C	1:A:342:THR:H	2.27	0.42
1:B:438:PHE:CE1	1:B:514:LYS:HD3	2.54	0.42
1:B:605:ASN:OD1	1:B:607:ASP:N	2.52	0.42
1:C:551:LEU:HB2	1:C:552:TRP:CE3	2.54	0.42
1:A:715:ASP:CG	1:A:718:ILE:HD13	2.44	0.42
1:B:364:TRP:HZ3	1:B:405:ILE:CD1	2.33	0.42
1:B:760:ASN:OD1	1:B:760:ASN:N	2.51	0.42
1:C:915:ILE:O	1:C:916:ALA:C	2.63	0.42
1:A:364:TRP:HZ3	1:A:405:ILE:CD1	2.33	0.42
1:B:595:LYS:HE2	1:B:595:LYS:HB3	1.83	0.42
1:C:152:LEU:O	1:C:153:ASN:HB2	2.20	0.42
1:C:335:GLN:NE2	1:C:908:TRP:NE1	2.64	0.42
1:A:71:ALA:O	1:A:75:ILE:HG12	2.20	0.42
1:A:739:ILE:O	1:A:741:ALA:N	2.52	0.42
1:B:29:ILE:HD13	1:B:109:ALA:HB1	2.01	0.42
1:B:322:ARG:HD3	1:B:322:ARG:H	1.84	0.42
1:B:523:VAL:O	1:B:555:LYS:NZ	2.48	0.42
1:C:378:VAL:HG21	1:C:753:MET:O	2.19	0.42
1:C:543:GLU:C	1:C:546:ASN:ND2	2.78	0.42
1:C:565:PRO:HD2	1:C:566:ARG:HD2	2.00	0.42
1:C:646:LYS:O	1:C:647:ARG:C	2.62	0.42
1:C:760:ASN:OD1	1:C:760:ASN:N	2.51	0.42
1:A:640:MET:HE3	1:A:640:MET:HB2	1.94	0.42
1:B:537:SER:CB	1:B:558:ASN:HB2	2.49	0.42
1:C:233:ILE:HD11	1:C:244:LEU:HB2	2.01	0.42
1:C:648:ILE:HD13	1:C:654:GLN:NE2	2.35	0.42
1:C:891:SER:O	1:C:893:LYS:N	2.53	0.42
1:B:171:ARG:HH11	1:B:171:ARG:CG	2.33	0.42
1:B:403:GLU:HG2	1:B:435:LEU:HD11	2.02	0.42
1:B:702:VAL:HG13	1:B:726:PHE:CE2	2.54	0.42
1:C:305:SER:O	1:C:309:GLN:HG3	2.19	0.42
1:C:777:ALA:O	1:C:778:ASN:C	2.62	0.42
1:A:413:ILE:HD11	1:A:432:MET:HE3	2.00	0.42
1:A:605:ASN:OD1	1:A:607:ASP:N	2.53	0.42
1:B:587:GLU:O	1:B:590:VAL:HG23	2.20	0.42
1:B:665:TYR:O	1:B:666:LYS:C	2.62	0.42
1:B:748:ILE:HB	1:B:793:PHE:HZ	1.85	0.42
1:B:758:THR:HB	1:B:762:LLP:H4'1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:SER:CB	1:B:762:LLP:OP3	2.67	0.42
1:C:62:ARG:HD2	1:C:191:TRP:O	2.20	0.42
1:C:739:ILE:O	1:C:741:ALA:N	2.53	0.42
1:C:748:ILE:HB	1:C:793:PHE:HZ	1.84	0.42
1:B:270:CYS:O	1:B:271:GLU:C	2.63	0.41
1:C:92:LEU:HD22	1:C:732:VAL:HG21	1.97	0.41
1:C:127:GLN:O	1:C:128:GLU:C	2.63	0.41
1:C:421:ASP:O	1:C:422:LEU:HB2	2.20	0.41
1:C:908:TRP:O	1:C:909:ASN:HB3	2.20	0.41
1:A:798:HIS:CE1	1:A:799:GLU:HG3	2.55	0.41
1:B:739:ILE:O	1:B:741:ALA:N	2.53	0.41
1:C:278:LYS:HA	1:C:281:TYR:CG	2.56	0.41
1:C:537:SER:C	1:C:540:VAL:HG12	2.46	0.41
1:C:549:TYR:O	1:C:553:PRO:HG3	2.20	0.41
1:C:788:GLU:OE1	1:C:788:GLU:HA	2.20	0.41
1:B:148:SER:O	1:B:149:LEU:C	2.63	0.41
1:B:570:ARG:HG3	1:B:570:ARG:HH11	1.85	0.41
1:C:548:PHE:O	1:C:551:LEU:CD2	2.69	0.41
1:C:777:ALA:O	1:C:780:GLU:N	2.52	0.41
1:B:278:LYS:HA	1:B:281:TYR:CG	2.56	0.41
1:B:305:SER:O	1:B:309:GLN:HG3	2.19	0.41
1:A:62:ARG:HD2	1:A:191:TRP:O	2.20	0.41
1:A:162:ARG:NH2	1:A:192:GLU:OE2	2.52	0.41
1:A:351:ILE:O	1:A:355:LEU:CG	2.65	0.41
1:A:438:PHE:CE1	1:A:514:LYS:HD3	2.56	0.41
1:B:639:ALA:HB1	1:B:682:PRO:C	2.46	0.41
1:B:777:ALA:O	1:B:778:ASN:C	2.63	0.41
1:C:151:THR:HG21	1:C:566:ARG:HH12	1.85	0.41
1:C:195:ARG:HB3	1:C:198:VAL:HG23	2.03	0.41
1:C:867:GLN:C	1:C:870:VAL:HG22	2.41	0.41
1:A:85:TYR:CE2	1:A:311:ILE:HG23	2.56	0.41
1:A:194:VAL:HG22	1:A:229:TYR:CE2	2.56	0.41
1:A:867:GLN:C	1:A:870:VAL:HG22	2.44	0.41
1:C:148:SER:O	1:C:149:LEU:C	2.63	0.41
1:C:598:GLU:O	1:C:601:LYS:HG2	2.21	0.41
1:C:695:TYR:O	1:C:696:VAL:C	2.63	0.41
1:C:759:SER:O	1:C:762:LLP:CG	2.69	0.41
1:A:695:TYR:O	1:A:696:VAL:C	2.64	0.41
1:A:758:THR:CB	1:A:762:LLP:H5'2	2.51	0.41
1:B:777:ALA:O	1:B:780:GLU:N	2.52	0.41
1:C:162:ARG:HB2	1:C:246:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ALA:HB1	1:C:335:GLN:HE22	1.85	0.41
1:C:547:ASP:O	1:C:550:GLU:HG2	2.20	0.41
1:A:152:LEU:O	1:A:153:ASN:HB2	2.20	0.41
1:A:270:CYS:O	1:A:271:GLU:C	2.63	0.41
1:A:598:GLU:O	1:A:601:LYS:HG2	2.21	0.41
1:A:759:SER:HB3	1:A:762:LLP:OP1	2.20	0.41
1:B:364:TRP:CH2	1:B:405:ILE:HG23	2.56	0.41
1:B:537:SER:OG	1:B:558:ASN:OD1	2.29	0.41
1:B:908:TRP:O	1:B:909:ASN:HB3	2.21	0.41
1:C:90:GLU:OE2	1:C:284:TYR:OH	2.31	0.41
1:C:152:LEU:HD11	1:C:154:TYR:CZ	2.49	0.41
1:C:605:ASN:OD1	1:C:607:ASP:N	2.53	0.41
1:A:520:ASN:O	1:A:524:VAL:HG23	2.21	0.41
1:B:324:LYS:O	1:B:327:GLU:HB2	2.21	0.41
1:B:85:TYR:CE2	1:B:311:ILE:HG23	2.56	0.40
1:B:385:LYS:HE2	1:B:436:GLU:OE1	2.22	0.40
1:C:548:PHE:N	1:C:551:LEU:CD2	2.83	0.40
1:A:82:LYS:HG3	1:A:331:LYS:C	2.47	0.40
1:A:517:ARG:HB2	1:A:520:ASN:HB2	2.03	0.40
1:B:695:TYR:O	1:B:696:VAL:C	2.63	0.40
1:B:769:ILE:HD12	1:B:880:TRP:CE2	2.57	0.40
1:C:151:THR:HG23	1:C:236:TYR:HB3	2.03	0.40
1:C:600:GLN:HG3	1:C:889:ALA:HB1	2.04	0.40
1:A:596:LEU:HB2	1:A:892:TYR:HB3	2.02	0.40
1:B:82:LYS:HG3	1:B:331:LYS:C	2.47	0.40
1:C:270:CYS:O	1:C:271:GLU:C	2.63	0.40
1:B:127:GLN:O	1:B:128:GLU:C	2.65	0.40
1:C:671:MET:SD	1:C:676:ARG:HG3	2.62	0.40
1:C:739:ILE:HB	1:C:740:PRO:HD3	2.03	0.40
1:B:136:GLY:O	1:B:137:GLY:C	2.65	0.40
1:B:623:VAL:HG22	1:B:737:LEU:HG	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	825/916 (90%)	744 (90%)	73 (9%)	8 (1%)	12	43
1	B	825/916 (90%)	744 (90%)	74 (9%)	7 (1%)	16	48
1	C	825/916 (90%)	744 (90%)	72 (9%)	9 (1%)	11	42
All	All	2475/2748 (90%)	2232 (90%)	219 (9%)	24 (1%)	12	43

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	381	GLU
1	B	381	GLU
1	C	381	GLU
1	C	388	TYR
1	A	47	ARG
1	C	47	ARG
1	A	441	PRO
1	A	618	SER
1	B	47	ARG
1	B	441	PRO
1	C	441	PRO
1	A	756	SER
1	C	756	SER
1	A	380	PRO
1	A	778	ASN
1	B	380	PRO
1	B	756	SER
1	B	778	ASN
1	C	380	PRO
1	C	778	ASN
1	B	155	PRO
1	A	155	PRO
1	C	155	PRO
1	C	323	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	707/786 (90%)	653 (92%)	54 (8%)	12	38
1	B	707/786 (90%)	662 (94%)	45 (6%)	16	43
1	C	707/786 (90%)	641 (91%)	66 (9%)	8	32
All	All	2121/2358 (90%)	1956 (92%)	165 (8%)	11	37

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	30	THR
1	A	47	ARG
1	A	64	SER
1	A	79	LEU
1	A	81	MET
1	A	209	SER
1	A	219	ILE
1	A	233	ILE
1	A	248	SER
1	A	251	VAL
1	A	273	GLN
1	A	275	ASN
1	A	297	LEU
1	A	321	ASP
1	A	322	ARG
1	A	323	ILE
1	A	353	ILE
1	A	355	LEU
1	A	365	ASN
1	A	377	THR
1	A	378	VAL
1	A	379	LEU
1	A	392	GLN
1	A	414	VAL
1	A	415	LEU
1	A	416	LYS
1	A	422	LEU
1	A	423	ASN
1	A	426	GLU
1	A	439	ASP

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Mol	Chain	Res	Type
1	A	444	VAL
1	A	517	ARG
1	A	527	HIS
1	A	543	GLU
1	A	587	GLU
1	A	617	ARG
1	A	636	VAL
1	A	646	LYS
1	A	648	ILE
1	A	651	TYR
1	A	676	ARG
1	A	697	GLN
1	A	712	ILE
1	A	718	ILE
1	A	748	ILE
1	A	758	THR
1	A	760	ASN
1	A	781	ILE
1	A	782	ARG
1	A	805	LYS
1	A	816	GLU
1	A	869	LYS
1	A	886	LEU
1	B	29	ILE
1	B	30	THR
1	B	46	GLU
1	B	47	ARG
1	B	79	LEU
1	B	81	MET
1	B	89	MET
1	B	171	ARG
1	B	209	SER
1	B	212	SER
1	B	219	ILE
1	B	233	ILE
1	B	248	SER
1	B	251	VAL
1	B	267	THR
1	B	270	CYS
1	B	275	ASN
1	B	297	LEU
1	B	323	ILE

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Mol	Chain	Res	Type
1	B	365	ASN
1	B	377	THR
1	B	381	GLU
1	B	392	GLN
1	B	414	VAL
1	B	415	LEU
1	B	422	LEU
1	B	423	ASN
1	B	426	GLU
1	B	444	VAL
1	B	511	ILE
1	B	587	GLU
1	B	600	GLN
1	B	636	VAL
1	B	646	LYS
1	B	647	ARG
1	B	651	TYR
1	B	676	ARG
1	B	677	LYS
1	B	683	ARG
1	B	701	ILE
1	B	750	THR
1	B	758	THR
1	B	760	ASN
1	B	813	VAL
1	B	905	LYS
1	C	29	ILE
1	C	30	THR
1	C	47	ARG
1	C	74	ASP
1	C	75	ILE
1	C	79	LEU
1	C	81	MET
1	C	89	MET
1	C	98	LEU
1	C	101	ILE
1	C	171	ARG
1	C	180	VAL
1	C	195	ARG
1	C	209	SER
1	C	219	ILE
1	C	233	ILE

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Mol	Chain	Res	Type
1	C	248	SER
1	C	251	VAL
1	C	267	THR
1	C	270	CYS
1	C	275	ASN
1	C	282	ILE
1	C	297	LEU
1	C	323	ILE
1	C	324	LYS
1	C	361	ASN
1	C	365	ASN
1	C	377	THR
1	C	381	GLU
1	C	392	GLN
1	C	414	VAL
1	C	415	LEU
1	C	422	LEU
1	C	423	ASN
1	C	426	GLU
1	C	439	ASP
1	C	444	VAL
1	C	511	ILE
1	C	538	GLU
1	C	543	GLU
1	C	548	PHE
1	C	551	LEU
1	C	566	ARG
1	C	587	GLU
1	C	596	LEU
1	C	598	GLU
1	C	599	LEU
1	C	616	LYS
1	C	636	VAL
1	C	646	LYS
1	C	647	ARG
1	C	651	TYR
1	C	664	ARG
1	C	669	LYS
1	C	676	ARG
1	C	677	LYS
1	C	742	SER
1	C	748	ILE

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Mol	Chain	Res	Type
1	C	750	THR
1	C	758	THR
1	C	760	ASN
1	C	781	ILE
1	C	782	ARG
1	C	788	GLU
1	C	813	VAL
1	C	848	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	153	ASN
1	A	299	GLN
1	A	375	ASN
1	A	527	HIS
1	A	530	ASN
1	A	546	ASN
1	A	654	GLN
1	A	697	GLN
1	A	747	HIS
1	A	770	GLN
1	A	834	ASN
1	B	153	ASN
1	B	299	GLN
1	B	375	ASN
1	B	527	HIS
1	B	530	ASN
1	B	654	GLN
1	B	747	HIS
1	B	834	ASN
1	B	845	ASN
1	C	123	ASN
1	C	153	ASN
1	C	335	GLN
1	C	368	GLN
1	C	375	ASN
1	C	527	HIS
1	C	530	ASN
1	C	536	HIS
1	C	546	ASN

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Mol	Chain	Res	Type
1	C	609	GLN
1	C	654	GLN
1	C	770	GLN
1	C	834	ASN
1	C	867	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	LLP	B	762	1	23,24,25	0.67	0	25,32,34	0.71	0
1	LLP	C	762	1	23,24,25	0.60	0	25,32,34	0.66	0
1	LLP	A	762	1	23,24,25	0.44	0	25,32,34	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	B	762	1	-	5/16/17/19	0/1/1/1
1	LLP	C	762	1	-	9/16/17/19	0/1/1/1
1	LLP	A	762	1	-	6/16/17/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	762	LLP	C5'-OP4-P-OP1
1	A	762	LLP	C5'-OP4-P-OP2
1	A	762	LLP	C5'-OP4-P-OP3
1	C	762	LLP	C5'-OP4-P-OP1
1	C	762	LLP	C5'-OP4-P-OP2
1	C	762	LLP	C5'-OP4-P-OP3
1	C	762	LLP	N-CA-CB-CG
1	C	762	LLP	C-CA-CB-CG
1	B	762	LLP	C4-C4'-NZ-CE
1	C	762	LLP	C4-C4'-NZ-CE
1	A	762	LLP	CD-CE-NZ-C4'
1	C	762	LLP	CE-CD-CG-CB
1	B	762	LLP	CE-CD-CG-CB
1	C	762	LLP	CG-CD-CE-NZ
1	C	762	LLP	CA-CB-CG-CD
1	B	762	LLP	CG-CD-CE-NZ
1	B	762	LLP	C3-C4-C4'-NZ
1	A	762	LLP	CE-CD-CG-CB
1	B	762	LLP	CA-CB-CG-CD
1	A	762	LLP	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	762	LLP	6	0
1	C	762	LLP	8	0
1	A	762	LLP	19	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	1101	-	5,5,5	0.16	0	5,5,5	0.20	0
2	GOL	C	1001	-	5,5,5	0.10	0	5,5,5	0.49	0
2	GOL	A	1102	-	5,5,5	0.08	0	5,5,5	0.35	0
3	CFF	C	1002	-	15,15,15	0.52	0	23,23,23	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	1101	-	-	1/4/4/4	-
2	GOL	C	1001	-	-	4/4/4/4	-
2	GOL	A	1102	-	-	2/4/4/4	-
3	CFF	C	1002	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

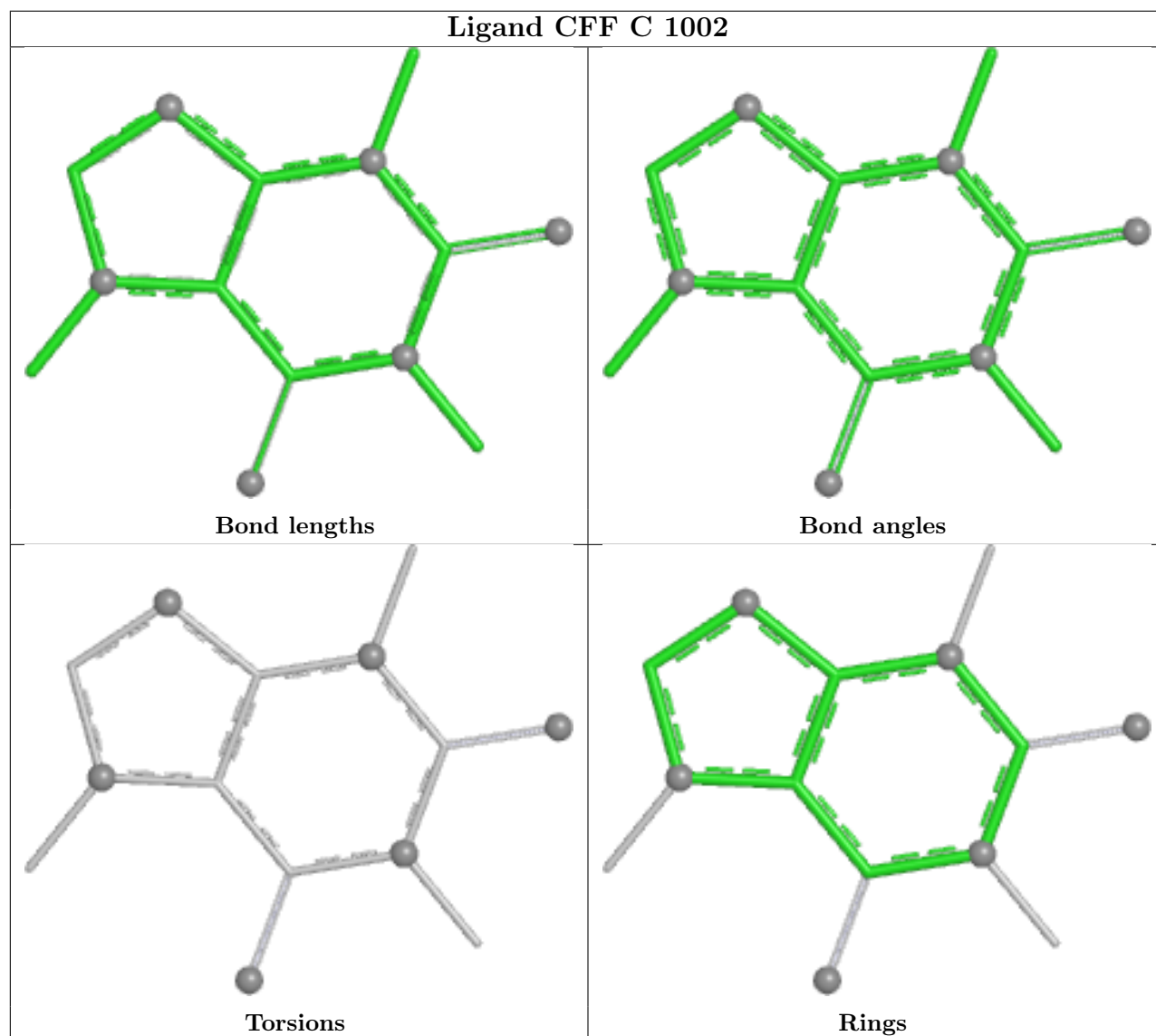
Mol	Chain	Res	Type	Atoms
2	A	1102	GOL	O1-C1-C2-C3
2	C	1001	GOL	O1-C1-C2-C3
2	C	1001	GOL	C1-C2-C3-O3
2	A	1102	GOL	O1-C1-C2-O2
2	C	1001	GOL	O1-C1-C2-O2
2	A	1101	GOL	O2-C2-C3-O3
2	C	1001	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	GOL	1	0
3	C	1002	CFF	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	829/916 (90%)	-1.24	0 100 100	26, 26, 26, 26	0
1	B	829/916 (90%)	-1.22	0 100 100	26, 26, 26, 26	0
1	C	829/916 (90%)	-1.20	0 100 100	26, 26, 26, 26	0
All	All	2487/2748 (90%)	-1.22	0 100 100	26, 26, 26, 26	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	LLP	A	762	24/25	0.99	0.06	26,26,26,26	0
1	LLP	B	762	24/25	0.99	0.04	26,26,26,26	0
1	LLP	C	762	24/25	0.99	0.05	26,26,26,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

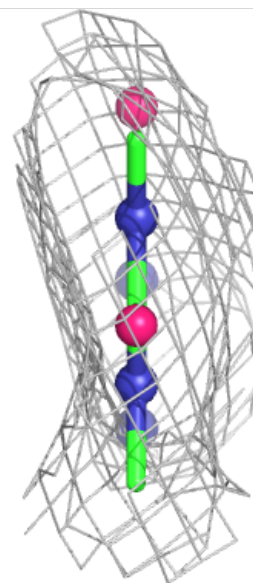
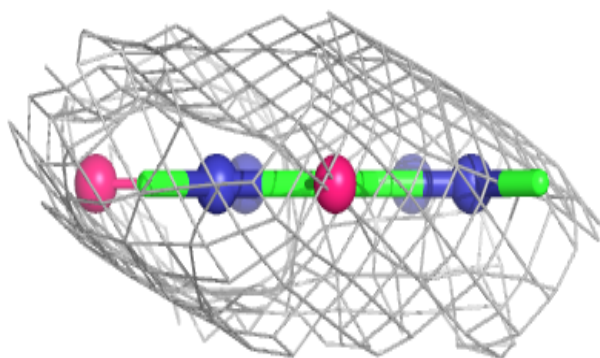
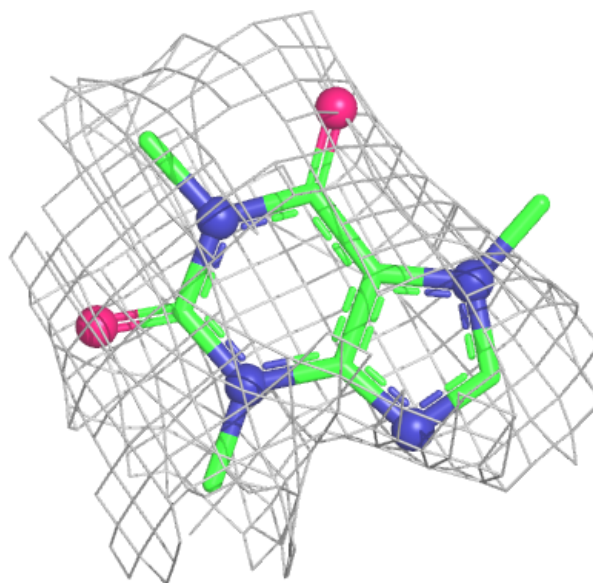
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	1102	6/6	0.96	0.07	47,47,47,47	0
2	GOL	C	1001	6/6	0.96	0.07	47,47,47,47	0
3	CFF	C	1002	14/14	0.97	0.10	47,47,47,47	0
2	GOL	A	1101	6/6	0.99	0.03	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CFF C 1002:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.